

CS205b/CME306

Lectures 1-1

1 Introduction

The goal of this class is to cover numerical simulation of PDEs, serving both the CME306 and CS205b groups, with the goal of changing the old CME306 style. The old CME306 went through compressible flow only, using that to dig into PDEs. Instead, this class is going to take a step back and think higher level about how to simulate fluids and solids, so we will not only look at the PDEs but also take a more general look at simulation for these systems that will have enough depth for the CME306 qualifying exam and yet have enough breadth that the students more interested in discrete math or CS get something more out of the class than just mathematical tools.

Because this is the second offering of the course, there will be no midterm or final. Note that ICME Ph.D. students will receive their qualifying exam on this material, so it may be advisable to work independently on homework as much as possible. This class is experimental, and we will be coming up with homework every week. We encourage you to ask a lot of questions, since the class is experimental and feedback will help us write the class. The homework for the class will be divided into a theory track and an application track. The theory track consists of purely written assignments (no programming) and will be relevant to the PDE qualifying exam, so it is recommended that ICME students that intend to take the qualifying exam take the theoretical option for their homework. The second homework track is a more applied track and will contain a mixture of theory and programming.

2 Simulation of Materials

2.1 Kinematic Description

One could abstractly consider chunks of mass moving around. Lets take the simplest chunks of mass, ones that do not have a lot of structure. For example, air particles moving around the room, or a chunk of mass could be a representative for a lot of air particles. The idea of a representative chunk is called a constituent model or an averaging model. Rather than simulating every particle or even atom, which is very expensive, one uses a chunk to represent many particles. Once one has these chunks of mass, what equations govern them? Each of these chunks may, for example, have a position x_i at any time and a mass m_i . The time derivative $u_i = x_i'$ tells how the chunks move around, and from there one can get an acceleration $a_i = u_i' = x_i''$. This gives some kinematic description of how the chunks move around so one can describe each chunk of mass separately. Once one has a description of the particles moving around, one can do an experiment with chunks moving around. Each chunk could be represented by any number of positions, and one typically uses the center of mass.

2.2 Conservation Laws

What things are true as the chunks move around? What are the governing equations? One typically thinks of these as the conservation laws: conservation of mass, momentum, and energy. These may become more complicated, such as adding viscosity to the momentum, thermal conductivity to the energy, or even relativistic effects, but in general there are guiding principles for these equations, which one can use to solve for the evolution of the chunks on a computer.

These governing equations can be written down differently depending on what one is doing. Some people write them down in what is called a Lagrangian form, and some write them down in what is called in an Eulerian form. The difference is whether the observer is sitting on a particle as it moves around (Lagrangian) or a sitting at a fixed location observing the particle as it moves (Eulerian).

As a 1D example, consider the conservation of mass per unit volume, where ρ is the density and u is the velocity,

$$\rho_t + (\rho u)_x = 0. \quad (1)$$

There are also strong and weak forms of this. The weak form of a PDE is expressed using integrals (but without spatial derivatives) with an equality enforced over some volume of space. The strong form is expressed using derivatives and can be obtained by eliminating the integrals from the weak form. We will get into this later in more detail. The second term is the flux term; it describes the rate of flow of material into and out of a region in space. Talk about why the sign should be positive. Expanding the spatial derivative yields

$$\rho_t + \rho_x u + \rho u_x = 0.$$

In this representation, the flux terms splits into two terms. The $\rho_x u$ term captures the change caused by a region of differing density moving across the current point. The ρu_x term captures the density change caused by material compressing or spreading out. This form of conservation of mass can be expressed using the material derivative as

$$\frac{D\rho}{Dt} + \rho u_x = 0, \quad (2)$$

where the material derivative is defined as

$$\frac{Df}{Dt} = f_t + u f_x.$$

Equation (2) looks more like the Lagrangian form. It is a time rate of change of the density, if you measure the density for a moving particle. The density change if moving with the flow is just based on the relative expansion near it. Equation (1) looks more like the Eulerian form and also takes account of the movement of the particle.

Somewhat more may be said about the material derivative. In higher dimensions, the material derivative may be defined as

$$\frac{Df}{Dt} = \frac{df}{dt} = \mathbf{p} f_t \frac{dt}{dt} + \sum_i \mathbf{p} f_{x_i} \frac{dx_i}{dt} = f_t + \mathbf{u} \cdot \nabla f.$$

The $\mathbf{u} \cdot \nabla f$ term (or $u f_x$ above) is referred to as an advection term and keeps track of the movement of the particle. It is written down explicitly in the Eulerian frame but not in the Lagrangian frame,

since it is implicitly included in the material derivative. We will look more at the Eulerian form later in the class, and for now we will focus on the Lagrangian form.

In the case of a Lagrangian frame, mass is attached directly to particles, such as in Figure 1, which are then evolved. As long as particles are not lost during the simulation, conservation of mass is obtained without future consideration. It will also transpire that conservation of energy may typically be ignored for Lagrangian simulations. The reason for this will become clear when deriving the incompressible equations, where we will show how the energy equation decouples from the other conservation laws.

$$m = \int_{-\infty}^{\infty} \rho(x) dx$$

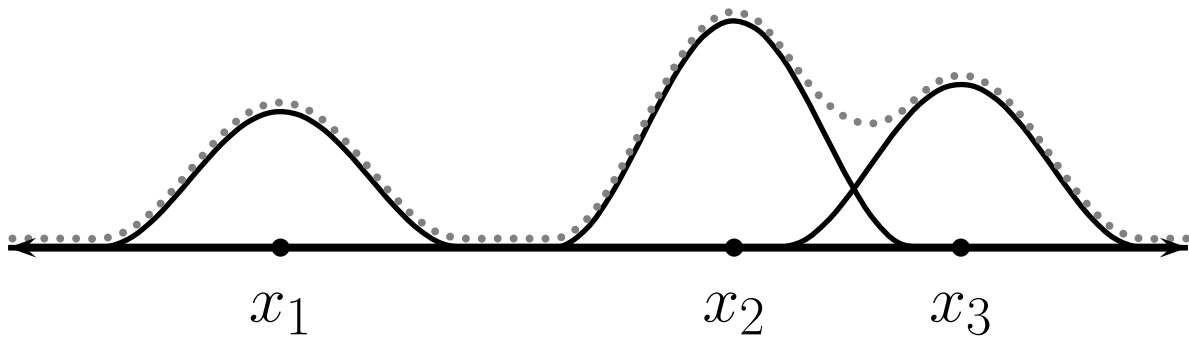


Figure 1: Three chunks located at x_1 , x_2 , and x_3 . The black curves show the density contribution of a single chunk at each point in space. The dotted line shows the density profile of space.